Electromagnetic Fields Scattered by Sub-Wavelength Sized Object of Drude Type Material in the Optical Region, Using a Finite Element Time Domain Method

Benedikt Oswald\textsuperscript{1,*} and Patrick Leidenberger\textsuperscript{2}

\textsuperscript{1} Paul Scherrer Institut (PSI), GFA, CH-5232 Villigen, Switzerland
\textsuperscript{2} Laboratory for Electromagnetic Fields and Microwave Electronics (IFH), Swiss Federal Institute of Technology Zurich (ETHZ), Gloriastrasse 35, CH-8092 Zurich, Switzerland

The concept of antennas has found renewed interest in near-field optics and the optics of nanometer-structured systems where dimensions are significantly smaller than the wavelength $\lambda$. Optical antennas usually consist of a combination of dielectric and metallic materials. Similar concepts are increasingly studied for nanometer-structured field-emission cathodes and field emitter arrays (FEA). They are used for time-resolved electron interferometry, imaging and for sources in particle accelerators where both single-tip emitters and FEA are currently studied. In this study we implement a finite element time domain (FETD) algorithm for the calculation of the electric field involving metals in the visible range of the electromagnetic spectrum, using a dispersive Drude dielectric model. We compute the distribution of the electric field for an optical antenna setup, consisting of a sharpened dielectric fiber tip and an attached gold nano-particle of sub-wavelength size, excited by an incoming plane wave from the negative $z$-axis that impinges onto the gold nanoparticle. We demonstrate the existence of spots of light of sub-wavelength dimensions, instrumental for circumventing the diffraction limit, i.e., to be able to detect objects smaller than about half the wavelength. We also model the coupling of the incoming plane wave into the dielectric fiber tip via the gold nano-particle. Finally, we demonstrate the importance of the finite element approach. Due to its inherent level of detail (LoD) it allows for the efficient discretization of configurations with a wide span of scales, from nanometer to micrometer, and, equally important, for the conformal and therefore more accurate discretization of curved geometrical features.

Keywords: Scattering, Electromagnetic, Sub-Wavelength Size, Drude Dispersive Dielectric, Finite Element Time Domain Method, FETD, Computational Electrodynamics, Field Emitter Arrays (FEA), Needle Cathodes.

1. INTRODUCTION

Recently, the concept of antennas has found renewed interest in near-field optics and the optics of nanometer-structured systems where dimensions are significantly smaller than the wavelength $\lambda$ of incoming or emitted light.\textsuperscript{1,4,29} Indeed, antenna shapes used in the microwave region have been revised and rescaled\textsuperscript{24} for applications in the visible, e.g., the butterfly shape, often used in microstrip techniques,\textsuperscript{11} has recently been studied.\textsuperscript{7,8,19} The dipole antenna was studied as one of the first\textsuperscript{12} whereas sphere-like particles and combinations thereof have been analyzed subsequently.\textsuperscript{13} In microwave engineering antennas are often conceptually considered as impedance transformers, converting the transmission line’s characteristic impedance, often 50 $\Omega$, to the free space impedance of 377 $\Omega$. The better this conversion is realized, the more power is radiated away from or received by the antenna; the efficiency of this process influencing the gain of the antenna. The gain expresses the ratio between the electric field radiated by the specific antenna and the field radiated by an isotropic, spherical radiator, denoted in units of decibel-isotropic, dBi, and depending on direction in a way that is characteristic for the specific antenna architecture.\textsuperscript{2} Then, in certain directions the electric field strength is considerably higher that in other directions. In the microwave region, antenna parameters are measured in the far-field of the radiating structure, i.e., at distances of at least a few $\lambda$ (practitioners use $5\lambda$ as rule-of-thumb) whereas in the case of optical antennas the distance between the ‘antenna’...
and the sample to be sensed are significantly smaller than the wavelength, usually a few nanometers only. While in the traditional, microwave, field of antenna engineering, the electromagnetic-field in the immediate vicinity of a radiation structure is not of primary interest and even avoided, in nano-optics it is the very near-fields that are of primary concern. The field close to a radiating dipole, aka. near-field, decays proportional to \( 1/r^3 \) where as the far-field decays proportional to \( 1/r \). This implies that the immediate near-field of a radiating structure can be used to sense sub-wavelength-sized structures due to the limited-size light spot. To design optical antennas therefore implies the analysis and optimization of the near-field distribution and intensity, especially to ensure as small a spot of light as possible, cf. Figure (1). Indeed, an object very close to the optical antenna influences the field distribution and therefore the signal detected or emitted.

Optical antenna concepts are also increasingly used for nanometer-structured field-emission cathodes; such emitters are currently of considerable interest for time-resolved electron interferometry, imaging and sources for particle accelerators. Both single-tip and field emitter arrays (FEA) are currently investigated. In particular, needle cathodes use similar tip shapes as apertureless scanning near-field optical microscopy (SNOM) instruments, e.g., Ref. [23], and are also made from metals, Zirconium–Carbide. The tip is illuminated with a laser of suitable wavelength \( \lambda \) while simultaneously a high voltage pulse is applied to the tip of the cathode, in order to lower the work function of the metal so that more electrons are emitted and the photocurrent increases. It has been found experimentally that the geometry of the tip strongly influences the photoemission. This is attributed to the fact that the tip’s shape determines the spatial variation of the quantum efficiency which eventually determines the emittance properties of the electron beam; the emittance of the electron gun being one of the key parameters of the X-ray free electron laser currently (PSI-XFEL) designed at the Paul Scherrer Institut (fel.web.psi.ch). This parameter influences the overall length of the accelerator in a decisive way. Therefore, considerable effort is currently being invested to design low emittance electron guns (LEG).

Common to both concepts, optical antennas and nanostructured photo emission cathodes, are:

(i) sub-wavelength features size, w.r.t. the illuminating laser;
(ii) illumination of the tip by laser light, from the visible to the infrared region of the spectrum;
(iii) particles attached to the tip; while to an optical antenna configuration a metal particle is deliberately attached.

The optical antenna consists of a dielectric fiber tip to which a gold nano-particle is attached. The fiber tip is modeled as a non-dispersive, linear isotropic dielectric. The gold nano-particle is modeled as a Drude material with parameters taken from Ref. [25]. The tip-particle configuration is illuminated by a plane wave propagating into the positive z-axis direction. We show the correspondence between the electric field and the geometry in the inset in the upper right corner. The nanoparticle corresponds to green-colored domain with ellipsoidal shape in the lower part of the field plot.

Fig. 1. The optical antenna consists of a dielectric fiber tip to which a gold nano-particle is attached. The fiber tip is modeled as a non-dispersive, linear isotropic dielectric. The gold nano-particle is modeled as a Drude material with parameters taken from Ref. [25]. The tip-particle configuration is illuminated by a plane wave propagating into the positive z-axis direction. We show the correspondence between the electric field and the geometry in the inset in the upper right corner. The nanoparticle corresponds to green-colored domain with ellipsoidal shape in the lower part of the field plot.
attached, at photocathodes, particles may appear as a result of the operation of the cathode, i.e., they are a parasitic consequence due to deformation of the cathode or even deposition of particles due to surface chemistry processes and thermal deformation.\textsuperscript{10} Nota bene, large current densities may arise during the operation of nanometer sized cathodes and cause ohmic losses.

In this study we focus on modeling the optical interaction between sub-wavelength sized tips and illumination by incoming laser light in the time domain. While nanoptics problems are often treated in the frequency domain\textsuperscript{3} applications of field-emitters\textsuperscript{14,30} indicate the generation of higher harmonics of the incoming laser pulse and therefore non-linear material properties which are more amenable for time-domain methods. In order to explore the electric field distribution we model the tip as a fully 3-dimensional structure, made from realistic material model, thereby ensuring that the tip–laser interaction model becomes more realistic.

2. FORMULATION OF THE PROBLEM

We compute the distribution of the electric field in the vicinity of a nanometer structured dielectric tip to which a sub-wavelength sized ellipsoidal gold particle is attached. The tip-particle configuration is illuminated by an incoming laser pulse which is modeled as a plane wave. The dielectric tip consists of a dielectric material with a low relative permittivity $\varepsilon_{\text{tip}}$ while the ellipsoidal particle is modeled with a Drude type, dispersive dielectric.\textsuperscript{25,33}

3. METHODS

We assume (i) isotropic, scalar material properties; (ii) non-dispersive magnetic permeability $\mu$; (iii) dispersive dielectric permittivity $\varepsilon$; (iv) a current density caused by ohmic conductivity $j_0 = \sigma E$; (v) an impressed current density $J$ which can be used to source the electromagnetic problem. Then, the electric field vector wave, aka. curl–curl, equation is given in the time domain\textsuperscript{16,34} by Eq. (1)

$$\nabla \times \left( \frac{1}{\mu} \nabla \times E + \sigma \frac{\partial}{\partial t} E + \frac{\partial^2}{\partial t^2} (\varepsilon \ast E) \right) = -\frac{\partial}{\partial t} J$$

where $E$ and $J$ both depend on space $r$ and time $t$.\textsuperscript{16,34} For solving Eq. (1) we use a finite element time domain (FETD) method,\textsuperscript{16} based on an extension of Ref. [27]. Here, we only describe the additional components of the finite element discretization that are required by the inclusion of a dispersive dielectric material model.

3.1. Drude Model

In the optical region of the electromagnetic spectrum metals are best approximated as imperfect, dispersive dielectric materials. The Drude model is often used in the frequency domain\textsuperscript{25} and given by Eq. (2)

$$\varepsilon_{\text{Drude}}(ω) = \varepsilon_\infty - \frac{\omega_p^2}{ω^2 - iω\gamma_p}$$

with $\varepsilon_\infty$ the permittivity at infinite frequency, $\omega_p$ the Drude pole frequency and $\gamma_p$ the inverse of the pole relaxation time. We note that the Drude model works best towards the red and infra-red region of the spectrum\textsuperscript{25} while towards the blue and ultra-violet (UV) region the addition of a Lorentz type model is required to provide sufficient accuracy. In this study we restrict ourselves to the Drude model. For time domain calculations we use the inverse Fourier transform of Eq. (2) and obtain\textsuperscript{21}

$$\varepsilon_{\text{Drude}}(t) = \varepsilon_\infty \delta(t) + \frac{\omega_p^2}{\gamma_p} \left( 1 - e^{-\gamma_p t} \right) U(t)$$

where $U(t)$ is the unit step, aka Heaviside, function. For integrating the Drude dispersive model into Eq. (1) we need to compute the 2nd time derivative of Eq. (3). Details of these calculations are given in Appendix 7.1. Eventually, we rewrite Eq. (1), using the operator defined in Eq. (39)

$$\mathcal{L}_{\text{Drude}}(E) \equiv \varepsilon_0 \omega_p^2 (1 - \gamma_p e^{-\gamma_p t} U(t) \ast) E$$

in compact form as

$$\nabla \times \frac{1}{\mu} \nabla \times E + \sigma \frac{\partial}{\partial t} E + \varepsilon_0 \varepsilon_\infty \frac{\partial^2}{\partial t^2} E + \mathcal{L}_{\text{Drude}}(E) = -\frac{\partial}{\partial t} J$$

(5)

where we note the introduction of a convolution operation in operator $\mathcal{L}$ due to the inclusion of the specific Drude dispersive dielectric material model from Eq. (3).

3.2. Spatial Discretization

To solve the dispersive curl–curl Eq. (5) we extend the finite element algorithm that has been developed earlier.\textsuperscript{27} In order to truncate the discretization of the computational domain, we use the 1st order absorbing boundary condition\textsuperscript{16} (pp. 530)

$$\hat{n} \times \left( \frac{1}{\mu} \nabla \times E \right) + \frac{1}{Z} \frac{\partial}{\partial t} \hat{n} \times (\hat{n} \times E) = U$$

(6)

where $\hat{n}$ denotes the outwards pointing unit normal vector on the boundary $S_o$ of the computational domain and $U$ corresponds to the time derivative of the tangential component of an impressed magnetic field. We will use $U$ to excite the electromagnetic problem through an incoming plane wave source. $Z$ is the impedance of the space that immediately borders the computational domain. The first term on the l.h.s. relates to the first time derivative of a tangential $H$-field that is rotated $90^\circ$ in space. The second term on the l.h.s. is the first time derivative of a tangential $E$-field. Thus, we obtain normally outgoing electric and magnetic fields, orthogonal to each other. This is equivalent to an outgoing plane wave, enforced on the boundary $S_o$.

3.2.1. Galerkin Approach

To solve Eq. (5) with a FE approach we approximate the unknown electric field $E$ within each element of the
mesh through a superposition of base functions \( w_j \) of
known shape but yet unknown scaling coefficients \( h_j \), aka.
degrees-of-freedom (DoF).

\[
E = \sum_j h_j w_j
\]  

(7)

The base functions \( w_j \) have compact support, i.e., they are
different from 0 only within their specific element. This
fact is relevant with respect to the structure of the sys-
tem matrices resulting from the discretization: the matrices
are sparse. There are two different ways to derive the lin-
ear system that determines the DoF from the vector wave
Eq. (5): (i) the variational approach\(^{16}\) and (ii) the weighted
residual approach.\(^{34}\) Both approaches eventually lead to

\[
\text{a function:}
\]

\[
\text{Eq. (5): (i) the variational approach}^{16} \text{and (ii) the weighted}
\]

\[
\text{residual approach.}^{34}
\]

\[
\text{both approaches eventually lead to}
\]

With these expansions we write the first integral as a func-
tion of \( \psi_j^{n-1} \):

\[
\psi_j^n = e^{-\gamma_j \Delta t} \psi_j^{n-1} + e^{-\gamma_j (n-1) \Delta t} \int_{(n-1) \Delta t}^{n \Delta t} e^{\gamma_j t'} h_j(t') dt'
\]  

(17)

The remaining integral in Eq. (17) can be calculated in
two different ways: using the trapezoidal rule, or assum-
ing \( h_j(t') \) to be a linear function on \((n-1)\Delta t \leq t' \leq n \Delta t\)
and integrate this analytically. The trapezoidal rule
evaluation is not used here due to insufficient accuracy.

A prohibitively small timestep would be required, slowing
considerably and rendering them useless in practice. A more
accurate evaluation of the integral in Eq. (17), thus avoiding
very small timesteps, can be achieved with an analytic reformulation.\(^{31}\) We assume

\[
h_j(t') = a_j^n t' + b_j^n, \quad (n-1) \Delta t \leq t' \leq n \Delta t
\]  

(18)

with slope \( a_j^n \) and intercept \( b_j^n \). We implement the convolution

\[
\text{3.2.2. Piecewise Linear Recursive Convolution (PLRC)}
\]

We implement the convolution \( e^{-\gamma_j t'} U(t') \ast h_j(t) \) efficiently
using a recursive approach.\(^{16,20}\) First, we reformulate
Eq. (10) using the properties of Heaviside’s unit step function:

\[
\psi_j(t) = e^{-\gamma_j t} U(t) \ast h_j(t) = \int_{-\infty}^{t} e^{-\gamma_j (t-t')} U(t-t') h_j(t') dt'
\]  

(11)

Now we rewrite Eq. (11), discretized in time:

\[
\psi_j^n = \psi_j(t)|_{t_n}
\]  

(12)

\[
= \int_{-\infty}^{n \Delta t} e^{-\gamma_j (n \Delta t-t')} h_j(t') dt'
\]  

(13)

\[
= \int_{-\infty}^{n \Delta t} e^{-\gamma_j n \Delta t} e^{\gamma_j t'} h_j(t') dt'
\]  

(14)

\[
J. \text{Comput. Theor. Nanosci. 6, 784–794, 2009}
\]  

787
and after inserting Eq. (23) into Eq. (17) we obtain
\[ \psi_j^h = e^{-\gamma_s\Delta t}\psi_j^{h-1} + \frac{1}{\gamma_p} (h_j^h - e^{\gamma_s\Delta t}h_j^{h-1}) \]
\[ - \frac{1}{\gamma_p} \frac{h_j^h - h_j^{h-1}}{\Delta t} (1 - e^{-\gamma_s\Delta t}) \] (24)

With this rearrangement we can calculate \( \psi_j^h \) accurately from \( \psi_j^{h-1} \) and the degree of freedom vectors \( h^h \) and \( h^{h-1} \). There is no need to save the total history of \( h(t) \) which results in considerable memory savings. The recursive convolution is implemented as shown in Eq. (24) in our code. The linear interpolation in Ref. [16, p. 551] is not the PLRC, but the simple trapezoidal rule as shown in Eq. (17). We emphasize the importance of the precise evaluation of the recursive convolution integral because we miss such a statement in the current literature.16

3.3. Time Discretization

For the time discretization of Eq. (9) we use a scheme based on central differences,16 accurate to 2nd order, and

\[ \psi_j^{h+1} = \frac{1}{1 + \frac{\Delta t}{\Delta t}} \psi_j^h + \frac{\Delta t}{1 + \frac{\Delta t}{\Delta t}} h_j^{h+1} - S h_j^{h+1} - Z \psi_j^{h+1} \]

We show a cut through the tetrahedral, computational mesh parallel the \( yz \)-plane. The mesh has been created with a focus on the level of detail (LoD) required by the structural properties of the optical antenna. In particular, the mesh exhibits relatively small tetrahedra around the gold nano-particle in order to accurately model the spherical particle shape. The capability of discretizing the curl-curl equation on a conformal grid is a decisive advantage of the finite element approach. In contrast, a traditional FDTD method will lead to a considerable computational and memory overhead in order to guarantee sufficient accuracy when resolving the ellipsoidal geometry of the gold nano-particle.17

4. RESULTS

For demonstrating the capability of the FETD approach we calculate the electric field of an optical antenna. The
antenna consists of a cone-shaped dielectric fiber tip to which a gold nano-particle of ellipsoidal shape has been attached. Both components are surrounded by vacuum. The configuration is shown in Figure 1 and its dimensions are given in Table I. The antenna is illuminated with a plane wave whose \( k \) vector impinges onto the gold particle from the negative \( z \)-axis direction. The polarization vector, i.e., \( \mathbf{E} \), is parallel to the \( y \)-axis. The dielectric fiber tip is modeled with a linear, isotropic, non-dispersive loss free permittivity. The gold nano-particle is modeled with a Drude type, linear, dispersive dielectric whose parameters are given in Table I and have been taken from\(^2\)

\(^2\) originally. If the particle was modeled as a perfect electrical conductor (PEC) the essential physics of the system would be missed. We have generated the finite element mesh using the \textit{tetgen} Delaunay based tetrahedral mesher.\(^1\)\(^2\) A specifically useful \textit{tetgen} feature is its capability to impose a shape quality criterion and an upper limit to the maximum acceptable volume of a tetrahedron. Thereby, precise control on mesh size in terms of numbers of tetrahedra is possible. We plot the cross section cut through the mesh and superimpose the calculated electric field

\begin{equation}
\text{(a) Simulated time } t = 2 \text{ fs}
\end{equation}

\begin{equation}
\text{(b) Simulated time } t = 4 \text{ fs}
\end{equation}

\begin{equation}
\text{(c) Simulated time } t = 6 \text{ fs}
\end{equation}

\begin{equation}
\text{(d) Simulated time } t = 8 \text{ fs}
\end{equation}

\begin{equation}
\text{(e) Simulated time } t = 10 \text{ fs}
\end{equation}

\begin{equation}
\text{(f) Simulated time } t = 12 \text{ fs}
\end{equation}

\begin{equation}
\text{(g) Simulated time } t = 14 \text{ fs}
\end{equation}

\begin{equation}
\text{(h) Simulated time } t = 16 \text{ fs}
\end{equation}

\begin{equation}
\text{(i) Simulated time } t = 18 \text{ fs}
\end{equation}

\textbf{Fig. 3.} Electric field magnitude, at \( t = 2, 4, 6, 8, 10, 12, 14, 16, 18 \text{ fs} \), in \text{dB}. The color scale of the snapshots is adapted to the electric field magnitude of the specific timestep. We observe light spots, of significantly smaller extent than the wavelength \( \lambda \), close to the gold nano-particle, that occur well in advance of the ‘bulk’ of the incoming plane wave. The light spots imply the existence of zones of electric field enhancement. Usually, structures smaller than about half the wavelength \( \lambda \) can not be detected due to the diffraction limit.\(^6\) Using the electromagnetic near-field is one approach to circumvent this restriction.\(^2\) In the case of optical antennas the detection of sub-wavelength sized objects exploits these sub-wavelength sized light spots.

Fig. 4. We plot the electric field magnitude, at \( t = 8, 10, 12, 14 \) and \( 16 \) fs, in dB. The color scale of the snapshots is adapted to the electric field magnitude of the specific timestep. In particular, we observe light spots close to the gold nano-particle, particularly in Figures 4(a, b, e and f); cf. also the "gremlin" like light spots in the lower part of Figure 2. The light spots imply the existence of zones of electric field enhancement; we note that the field enhancement occurs well in advance of the 'bulk' of the incoming plane wave. The spots constitute a field that is similar a radiating dipole, indicating a separation of charge that induces a dipole and its associated electric field lines.\(^7\) W.r.t detecting sub-wavelength sized objects the comments in Figure 3 also apply.
Oswald and Leidenberger Electromagnetic Fields Scattered by Sub-Wavelength Sized Object of Drude Type Material

in order to show the correspondence between level of detail and electric field distribution features in Figure 2. In Figure 3 we show the evolution of the electric field, i.e., its magnitude sampled on $x_2$ and $y_2$ cut planes, in logarithmic scale. The plane wave impinges onto the gold nanoparticle from the negative $z$-direction with the polarization vector $p$ along the $y$-axis. The color scale of the snapshots is adapted to the electric field magnitude of the specific timestep. In Figure 4 we show the evolution of the electric field, i.e., its magnitude sampled on the $yz$ and parts of the $xy$ plane. The $x_2$ cut plane has been laid through the equatorial plane of the gold nano-particle. Again, the color scale of the snapshots is adapted to the electric field magnitude of the specific timestep. These plots have been inserted in order to demonstrate the field enhancement that arises in the immediate vicinity of the gold nano-particle, well in advance of the ‘bulk’ of the incoming plane wave. In Figure 4(f) a Hertzian dipole like field pattern is clearly visible.

5. DISCUSSION

The electric field distribution of a optical antenna configuration, illuminated by a plane wave, has been calculated. While the gold nano-particle, attached to the dielectric tip, is considerably smaller than the wavelength $\lambda$ of the incoming plane wave, the electric field nevertheless shows distinctive features that are commensurate with the dimension of the nanoparticle, nota bene. We note that the size of the tetrahedral elements during the mesh generation phase is closely linked to these features’ size. While a usual rule of thumb requires a mesh size corresponding, roughly, to $\lambda/10$ or $\lambda/20$ this is not sufficient here; rather we are in a regime where mesh size tends to become $\lambda/100$ or even smaller; in particular this is the case in the vicinity of the gold nano-particle, Figure 2. Such small mesh dimensions can easily lead to prohibitive requirements w.r.t. computation time and memory. In particular, if a discretization relies on cartesian orthogonal grids, where the size of the smallest feature determines the size of the mesh as e.g., in finite-difference time-domain (FDTD) methods.\textsuperscript{17, 31} From another point of view, if the size of features $\lesssim \lambda$, the size of the computational mesh must be selected accordingly in order to accurately resolve the essential physics of the system.

In Figures 3 and, particularly, 4 we observe light spots, close to the surface of the gold nano-particle, aligned with the polarization vector $p$. These domains are significantly smaller than the wavelength. The lateral dimension is roughly on the order of 60 to 70 nm. These light spots constitute a field that is similar to the field of a radiating dipole, indicating a separation of charge that induces a dipole and its associated electric field lines.\textsuperscript{5} Because gold in the optical region of the spectrum is not a PEC material but more a Drude type dispersive dielectric\textsuperscript{31} the field inside the gold nano-particle will not be zero. When the plane wave impinges onto the gold nano-particle it is therefore not just reflected as in the case of a PEC material but it penetrates the metal and propagates within, albeit attenuated. Further, these light spots imply the existence of zones of electric field enhancement, cf. particularly Figures 4(a, b, and f). Through out the transition of the plane wave these light spots exist; although they change their shape. Usually, structures smaller than about half the wavelength $\lambda$ can not be detected due to the diffraction limit.\textsuperscript{6} Using the electromagnetic near-field is one approach to circumvent this restriction.\textsuperscript{25} Therefore, the existence of light spots smaller than the wavelength $\lambda$ is instrumental. In the case of optical antennas the detection of sub-wavelength sized objects exploits these sub-wavelength sized light spots. Also, in Figures 4(d and e) we observe how the plane wave is coupled via the gold nano-particle into the dielectric fiber tip and propagating inside it towards the positive $z$-axis. In particular, in Figure 4(e) we observe how part of the field, that propagates inside the tip, is radiated away from the sides of the tip and therefore will not contribute to the signal detected at the end of the fiber.

6. SUMMARY AND CONCLUSIONS

We have implemented an algorithm for the calculation of the time-dependent electric field for modeling dispersive Drude type dielectric materials in the time domain. This has been motivated by the need to model metals in the visible part of the electromagnetic spectrum where they do not behave as pure metals but must be treated as imperfect, lossy, dispersive dielectrics. We have computed the distribution of the electric field for an antenna setup, consisting of a combination of sharpened dielectric fiber tip and a gold nano-particle of subwavelength size, excited by an incoming plane wave from the negative $z$-axis that impinges onto the gold nano-particle. We were able to demonstrate the existence of spots of light of sub-wavelength dimensions, instrumental for circumventing the diffraction limit, i.e., to be able to detect objects smaller than about half the wavelength. Also, the calculation have shown that part of the incoming plane wave is coupled into the dielectric fiber tip via the gold nano-particle. This is relevant for the detection of signals sensed by the optical antenna in the sense that it demonstrates the suitability of the setup. Our algorithm therefore forms the basis for further analysis and optimization of optical antenna structures which will also become increasingly important building blocks for nano-structured field emitter arrays, i.e., photo cathodes for accelerators and electron microscopes. In the case of photo cathodes, in order to have a complete model, electron emission and thermal effects will eventually be required. In order to more accurately model metals at shorter visible wavelengths and
7. APPENDIX

7.1. Reformulating the Drude Model

We apply the rule of differentiation to the convolution integral
\[ e^{-\gamma' t} \delta(t) * E(t) = \int_{-\infty}^{\infty} e^{-\gamma' t'} \delta(t - t') dt' \]
\[ = E(t) \quad (28) \]

We now have
\[ \frac{\partial^2}{\partial t^2}(\epsilon_0 \epsilon_r(t) * E) = \epsilon_0 \frac{\partial^2}{\partial t^2}(\delta(t) * E) \]
\[ = \epsilon_0 \alpha_p^2 \frac{\partial^2}{\partial t^2}((1 - e^{-\gamma' t'})U(t) * E) \quad (30) \]

We subdivide the application of the time derivative into two parts, with the first part
\[ \epsilon_0 \frac{\omega_p^2}{\gamma_p} \frac{\partial^2}{\partial t^2}((1 - e^{-\gamma' t'})U(t) * E) \]
\[ = -\epsilon_0 \frac{\omega_p^2}{\gamma_p} \frac{\partial}{\partial t}((1 - e^{-\gamma' t'})U(t) * E) \]
\[ = -\epsilon_0 \frac{\omega_p^2}{\gamma_p} \frac{\partial}{\partial t}(-\gamma_p e^{-\gamma' t}U(t) + e^{-\gamma' t} \delta(t)) * E \]
\[ = -\epsilon_0 \frac{\omega_p^2}{\gamma_p} \frac{\partial}{\partial t}(-\gamma_p e^{-\gamma' t}U(t) * E - \epsilon_0 \frac{\partial^2}{\partial t^2} \frac{\partial}{\partial t} U(t) * E) \]
\[ = -\epsilon_0 \frac{\omega_p^2}{\gamma_p} \frac{\partial}{\partial t}(-\gamma_p e^{-\gamma' t}U(t) * E) \quad (33) \]

We note that the last term in Eq. (34) cancels out the first part, Eq. (31) and therefore, it remains to simplify what remains from Eq. (34) through consolidating signs and evaluating the time derivative.\[
\frac{-\epsilon_0 \omega_p^2}{\gamma_p} \frac{\partial}{\partial t}(-\gamma_p e^{-\gamma' t}U(t) * E) \]
\[ = \epsilon_0 \omega_p^2 \frac{\partial}{\partial t}(e^{-\gamma' t}U(t) * E) \quad (35) \]

and upon using Eq. (28) we obtain for the second part of Eq. (30)
\[ \frac{-\epsilon_0 \omega_p^2}{\gamma_p} \frac{\partial}{\partial t}(-\gamma_p e^{-\gamma' t}U(t) * E) \]

Eventually, the variable, i.e., time-dependent, part of the Drude dispersive dielectric model becomes
\[ \frac{\partial^2}{\partial t^2}(\epsilon_0 \epsilon_r(t) * E) = \epsilon_0 \alpha_p^2 ((1 - \gamma_p e^{-\gamma' t}U(t)) * E) \quad (38) \]

which is condensed into an operator
\[ \mathcal{F}_{\text{Drude}}(E) \quad (39) \]

7.2. Derivation of the Spatial Discretization

Here we derive the finite element discretization of the electric-field vector wave Eq. (5) using the weighted residual approach.\[ \int \int \int \left( \nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} + \sigma \frac{\partial \mathbf{E}}{\partial t} \right) \mathbf{J} \, dV = 0 \quad (40) \]

The double curl expression in Eq. (5) \( \nabla \times 1/\mu \nabla \times \mathbf{E} \), requires base functions that are at least twice differentiable. To relax these requirements we reformulate it using the first of Green’s vector theorems:16 (p. 711)
\[ \int \int \int u(\mathbf{a} \times \nabla \times \mathbf{b}) \, dV = \int \left( \int \mathbf{a} \cdot (\nabla \times \mathbf{v}) \cdot \mathbf{n} \, dS \right) \quad (41) \]

We set \( u = 1/\mu, a = \mathbf{t}, \) and \( b = \mathbf{E} \) and applying Eq. (41) onto Eq. (40) we obtain the so-called weak formulation, because the double curl expression has been brought into a more balanced formulation
\[ \int \int \int \left( \frac{1}{\mu} (\nabla \times \mathbf{t}) \cdot (\nabla \times \mathbf{E}) + \sigma \frac{\partial \mathbf{E}}{\partial t} \right) \mathbf{J} \, dV \]
\[ = \int \int \int \left( \frac{1}{\mu} (\mathbf{t} \times \nabla \times \mathbf{E}) \cdot \mathbf{n} \, dS \right) \quad (42) \]

The 1st order ABC will be integrated into the weak formulation via the surface integral we obtain inserting Green’s vector theorem Eq. (41). The surface over which we integrate is the computational domain’s surface. We use the fundamental vector identities
\[ \mathbf{t} \times (\nabla \times \mathbf{E}) \cdot \mathbf{n} = \mathbf{n} \cdot (\mathbf{t} \times \nabla \times \mathbf{E}) = \mathbf{t} \cdot (\nabla \times \mathbf{E} \times \mathbf{n}) \]
\[ = -\mathbf{t} \cdot (\mathbf{n} \times \nabla \times \mathbf{E}) \quad (43) \]
Electromagnetic Fields Scattered by Sub-Wavelength Sized Object of Drude Type Material

applying it to Eq. (42) and obtain
\[
\iiint_v \left( \frac{1}{\mu} (\nabla \times \mathbf{t}) \cdot (\nabla \times \mathbf{E}) + \mathbf{t} \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dV + \iiint_v \left( \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} + \mathbf{t} \cdot \frac{\partial \mathbf{J}_\text{ext}}{\partial t} \right) dV + \iiint_v (\mathbf{t} \cdot \nabla \cdot \mathbf{E}) dV = 0
\]

with a reformulation of the ABC Eq. (6)
\[
\frac{1}{\mu} \mathbf{n} \times \nabla \times \mathbf{E} = \mathbf{U} - \frac{1}{Z} \frac{\partial}{\partial t} (\mathbf{n} \times \mathbf{E})
\]

we obtain
\[
\iiint_v \left( \frac{1}{\mu} (\nabla \times \mathbf{t}) \cdot (\nabla \times \mathbf{E}) + \mathbf{t} \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dV + \iiint_v \left( \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} + \mathbf{t} \cdot \frac{\partial \mathbf{J}_\text{ext}}{\partial t} \right) dV + \iiint_v (\mathbf{t} \cdot \nabla \cdot \mathbf{E}) dV = 0
\]

Using a further vector identity
\[
\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a}
\]
we can reformulate the second term in the surface integral:
\[
\mathbf{t} \cdot (\mathbf{n} \times (\mathbf{n} \times \mathbf{E})) = (\mathbf{n} \times \mathbf{E}) \cdot (\mathbf{t} \times \mathbf{n}) = (\mathbf{t} \times \mathbf{n}) \cdot (\mathbf{n} \times \mathbf{E}) = - (\mathbf{n} \times \mathbf{t}) \cdot (\mathbf{n} \times \mathbf{E})
\]

We insert this into Eq. (46), considering that \( \mathbf{t} \) and \( \mathbf{n} \) are not time dependent, we obtain
\[
\iiint_v \left( \frac{1}{\mu} (\nabla \times \mathbf{t}) \cdot (\nabla \times \mathbf{E}) + \mathbf{t} \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dV + \iiint_v \left( \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} + \mathbf{t} \cdot \frac{\partial \mathbf{J}_\text{ext}}{\partial t} \right) dV + \iiint_s \left( \mathbf{t} \cdot \mathbf{U} + \frac{1}{Z} (\mathbf{n} \times \mathbf{t}) \cdot \frac{\partial}{\partial t} (\mathbf{n} \times \mathbf{E}) \right) dS = 0
\]

The external current density term, modeling an impressed excitation, is shifted onto the right hand side:
\[
\iiint_v \left( \frac{1}{\mu} (\nabla \times \mathbf{t}) \cdot (\nabla \times \mathbf{E}) + \mathbf{t} \cdot \frac{\partial \mathbf{E}}{\partial t} + \mathbf{t} \cdot \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} \right) dV + \iiint_v (\mathbf{t} \cdot \nabla \cdot \mathbf{E}) dV + \iiint_s \left( \mathbf{t} \cdot \mathbf{U} + \frac{1}{Z} (\mathbf{n} \times \mathbf{t}) \cdot \frac{\partial}{\partial t} (\mathbf{n} \times \mathbf{E}) \right) dS = 0
\]

We further remember that \( \mathbf{E} \) is approximated element-wise by Eq. (7) in Eq. (50). Next, the testing function \( \mathbf{t} \) must be chosen. While there is a wide selection of eligible function spaces, most often the test function is selected from

the same family as the base functions \( \mathbf{w} \). If the test function originates from the same family, the weighted residual approach becomes the well-known Galerkin method.\(^{16,34} \)

We insert Eq. (7) into Eq. (50) and choose the test function \( \mathbf{t} = \mathbf{w} \). Additionally, we assume that the base functions depend on space only and the scaling coefficients \( h_j \) depend on time only. We obtain, when testing by all base functions \( \mathbf{w}_j \) associated with topological entities of the mesh:
\[
\iiint_v \left( \frac{1}{\mu} (\nabla \times \mathbf{w}_j) \cdot (\nabla \times \mathbf{E}) + \mathbf{w}_j \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dV + \iiint_v \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} dV + \iiint_v \mathbf{w}_j \cdot \frac{\partial \mathbf{J}_\text{ext}}{\partial t} dV + \iiint_v (\mathbf{w}_j \cdot \nabla \cdot \mathbf{E}) dV
\]

The evaluation of all combinations of base functions \( \mathbf{w}_i, \mathbf{w}_j \) produces the local, elemental matrices and the forcing vector whose expressions are:
\[
T_{ij} = \iiint_v \varepsilon_\infty \mathbf{w}_i \cdot \mathbf{w}_j dV \quad R_{ij} = \iiint_v \mathbf{w}_i \cdot \frac{\partial \mathbf{E}}{\partial t} dV \quad Q_{ij} = \iiint_v \frac{1}{\mu} (\nabla \times \mathbf{w}_i) \cdot (\nabla \times \mathbf{w}_j) dV \quad S_{ij} = \iiint_v (\nabla \cdot \mathbf{E}) \mathbf{w}_i \cdot \mathbf{w}_j dV \quad U_{ij} = \iiint_v \mathbf{w}_i \cdot \mathbf{w}_j dV \quad Z_{ij} = - \iiint_v \varepsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} dV \quad f_i = \iiint_v \mathbf{w}_i \cdot \frac{\partial \mathbf{J}_\text{ext}}{\partial t} dV + \iiint_s \mathbf{w}_i \cdot \mathbf{U} dS
\]

for the most part we follow the nomenclature adopted in Ref. [16]. Once the local element matrices have been assembled into the global matrix, we rewrite Eq. (51) as a system of linear, inhomogeneous ordinary differential equations
\[
T \frac{\partial^2 \mathbf{h}}{\partial t^2} + (R + Q) \frac{\partial \mathbf{h}}{\partial t} + (S + U) \mathbf{h} + Z \psi = - \mathbf{f}
\]
where \( T, R, Q, S, U, \) and \( Z \) denote the global finite element matrices, \( \mathbf{h} \) the global vector of degrees of freedom, \( \mathbf{f} \) the global forcing vector and \( \psi \) the convolution vector whose elements are
\[
\psi_j(t) = e^{-\gamma_j t} U(t) \ast h_j(t)
\]
Electromagnetic Fields Scattered by Sub-Wavelength Sized Object of Drude Type Material
Oswald and Leidenberger

Acknowledgments: The authors thank the anonymous reviewers for their thoughtful reviews.

References


Received: 9 October 2008. Accepted: 30 October 2008.